

Supporting information

Thermophysical Properties of Lithium Thiogallate that Are Important for Optical Applications

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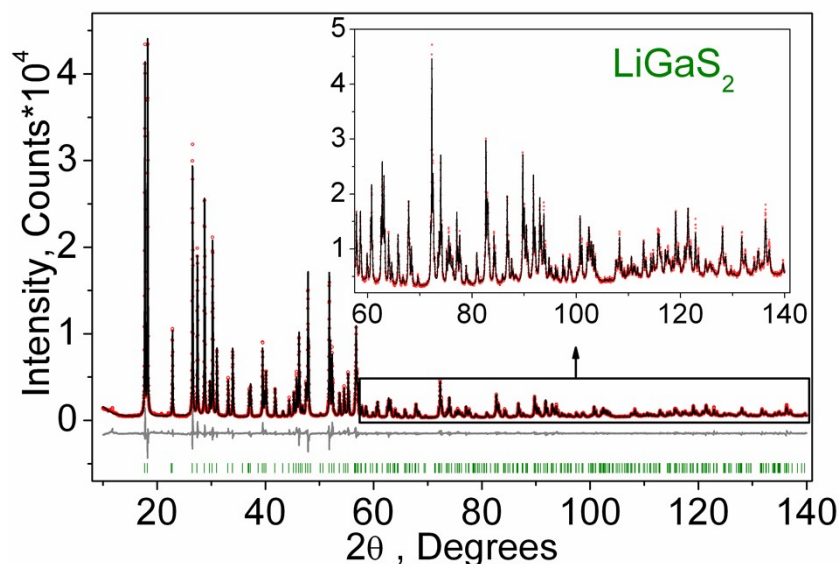


Figure S1. Difference Rietveld plot of LiGaS_2 . (red dots – experimental data y_o , black line – calculated pattern y_c , grey line below – difference $y_o - y_c$, green sticks below – positions of Bragg peaks) of LiGaSe_2 .

Table S1. Fractional atomic coordinates and isotropic displacement parameters (\AA^2) of LiGaS_2

	x	y	z	B_{iso}
Ga	0.0732 (1)	0.1262 (4)	0	0.56 (6)
Li	0.083 (2)	0.629 (5)	0.025 (3)	0.6 (3)
S1	0.0672 (3)	0.1165 (5)	-0.3654 (3)	0.86 (7)
S2	0.4026 (3)	0.1368 (5)	0.1176 (3)	0.86 (7)

Table S2. Main bond lengths (\AA) of LiGaS_2

Bond	Bond length, (\AA)	Bond	Bond length, (\AA)
Ga—S1	2.275 (2)	Li—S1 ⁱⁱⁱ	2.33 (4)
Ga—S1 ⁱ	2.276 (4)	Li—S1 ^{iv}	2.38 (1)
Ga—S2	2.269 (2)	Li—S2 ^v	2.54 (2)
Ga—S2 ⁱⁱ	2.290 (4)	Li—S2 ⁱⁱ	2.47 (3)

Symmetry codes: (i) $-x, -y, z+1/2$; (ii) $x-1/2, -y+1/2, z$; (iii) $-x, -y+1, z+1/2$; (iv) $-x+1/2, y+1/2, z+1/2$; (v) $-x+1/2, y+1/2, z-1/2$

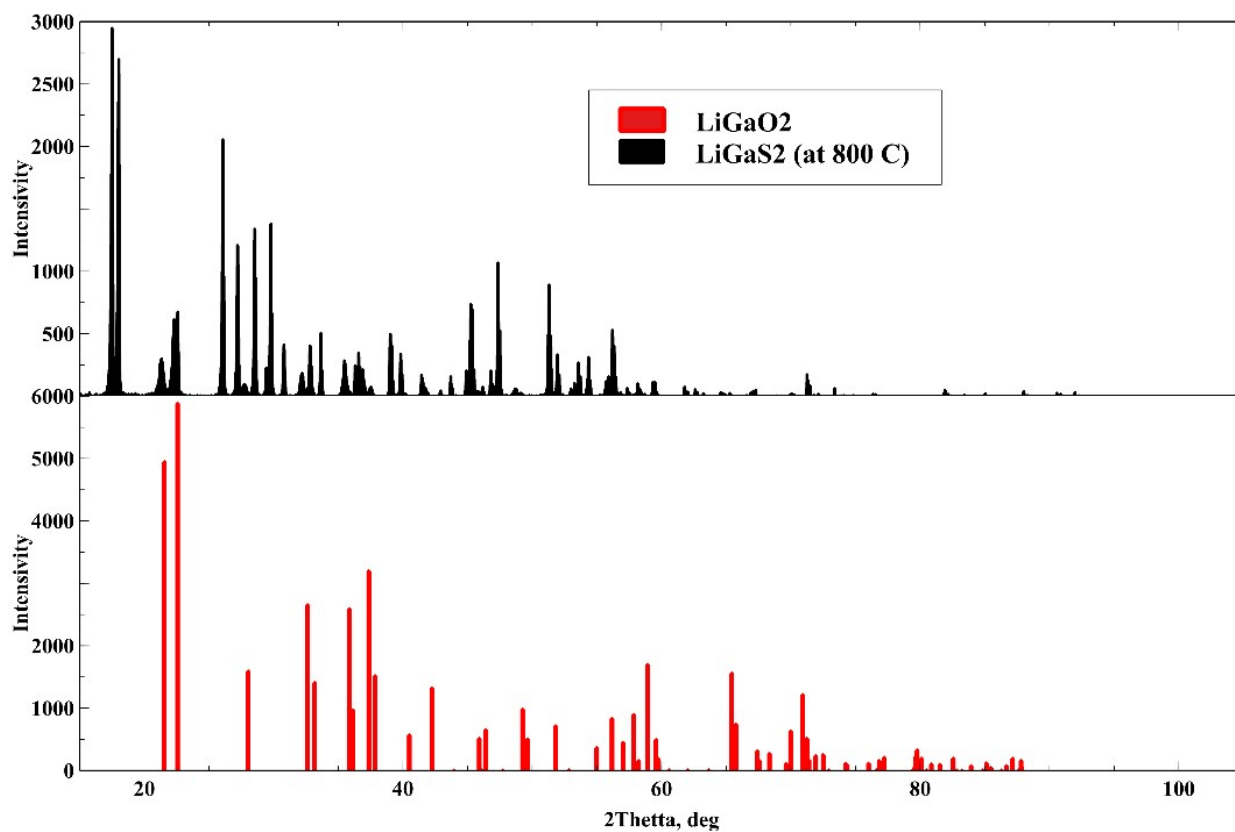


Figure S2. Comparison of the X-ray diffractograms for LiGaS₂ obtained at 1080 K (above) and LiGaO₂ (below, taken from [21]).